

Sebacic acid, isobutyl 3-phenylallyl ester

Inchi:	InChI=1S/C23H34O4/c1-20(2)19-27-23(25)17-11-6-4-3-5-10-16-22(24)26-18-12-15-21-1
InchiKey:	NPVLIHHTMWLZRP-NTCAYCPXSA-N
Formula:	C23H34O4
SMILES:	CC(C)COC(=O)CCCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]:	374.51

Physical Properties

Property code	Value	Unit	Source
gf	-134.87	kJ/mol	Joback Method
hf	-659.18	kJ/mol	Joback Method
hfus	51.62	kJ/mol	Joback Method
hvap	86.95	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.563		Crippen Method
mvol	321.750	ml/mol	McGowan Method
pc	1154.57	kPa	Joback Method
rinpol	2848.00		NIST Webbook
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tb	908.62	K	Joback Method
tc	1117.04	K	Joback Method
tf	499.63	K	Joback Method
vc	1.238	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.55	J/molxK	908.62	Joback Method
cpg	1102.50	J/molxK	1082.30	Joback Method
cpg	1090.52	J/molxK	1047.57	Joback Method
cpg	1077.48	J/molxK	1012.83	Joback Method
cpg	1063.34	J/molxK	978.09	Joback Method
cpg	1048.05	J/molxK	943.36	Joback Method
cpg	1113.49	J/molxK	1117.04	Joback Method
dvisc	0.0000280	Paxs	908.62	Joback Method

dvisc	0.0000375	Paxs	840.45	Joback Method
dvisc	0.0000528	Paxs	772.29	Joback Method
dvisc	0.0000794	Paxs	704.12	Joback Method
dvisc	0.0001304	Paxs	635.96	Joback Method
dvisc	0.0002413	Paxs	567.79	Joback Method
dvisc	0.0005281	Paxs	499.63	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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